## **Mathematical Modeling and Analysis**

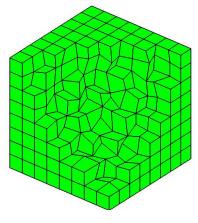


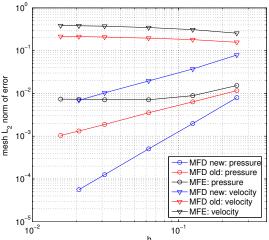
## New Discretization Methodology for Diffusion Problems on Polyhedral Meshes

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Tetrahedral and structured hexahedral meshes have been used for decades in a majority of engineering simulations; they are relatively easy to generate and there exists an enormous repository of numerical methods designed for these meshes. Nowadays, a growing number of complex simulations shows advantage of using polyhedral meshes. For example, in the simulation of flow through a water jacket of an engine [1], the results obtained on a polyhedral mesh are more accurate than the results obtained on a tetrahedral mesh with a comparable number of cells. In oil reservoir simulations, the polyhedral mesh topology offers unlimited possibilities: cells can be automatically joined, split, or modified by introducing additional points, edges and faces to model complex geological features. nately, most of the existing numerical methods cannot be extended to polyhedral meshes, especially to meshes with cells having strongly curved (non-planar) faces.

In [2], we considered a diffusion problem, which appears in computational fluid dynamics, heat conduction, radiation transport, etc., and developed a new discretization methodology that has no analogs in literature. The methodology follows the general principle of the mimetic finite difference (MFD) method — to mimic the essential underlying properties of the original continuum differential operators such as the conservation laws, solution symmetries, and the fundamental identities and theorems of vector and tensor calculus.





A logically cubic mesh (top picture) with randomly perturbed interior points. Part of the unit cube was cut out to show the interior mesh. The convergence graphs (bottom picture) for a smooth solution and the identity diffusion tensor show optimal convergence rates for the new MFD method (blue), and the lack of convergence for the mixed finite element (black) and the old MFD (red) methods.

The mixed form of the diffusion problem is

$$\vec{F} = -K \text{ grad } p, \qquad \text{div } \vec{F} = b$$

where the first equation is the constitutive equation relating the scalar function p (pressure in flow simulations) to the velocity field  $\vec{F}$  and the second one is the mass conservation law. The material properties are described by the full sym-

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metric tensor K, and b is the source function. For this problem, the MFD method mimics the Gauss divergence theorem, the symmetry between the continuous gradient and divergence operators, and the null spaces of these operators. Therefore, it produces the discretization scheme which is symmetric and locally conservative.

The old MFD method [3] used one degree of freedom per cell to approximate the pressure and one degree of freedom per mesh face to approximate the average normal component of the velocity. The same degrees of freedom are used in the mixed finite element method on tetrahedral and hexahedral meshes.

The new discretization methodology [2] uses three degrees of freedom, three average velocity components, to approximate velocity on strongly curved faces. It results in the new MFD method that improves drastically the capabilities of the existing methods (see figures). When faces of mesh cells are plane segments, or slightly perturbed plane segments, the new MFD method is reduced to the old one from [3]. When the faces are strongly curved, the extra degrees of freedom allow the new method to succeed and perform much better than other methods. The theoretical analysis of the new method is done in [2].

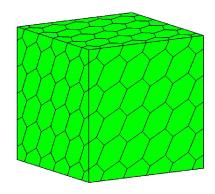
Another advantage of the developed methodology is that its practical implementation is simple and follows roughly the path described in [4]. In particular, we get a family of discretization schemes with similar properties. This family of schemes may be used to tackle other computational problems such as enforcement of the discrete maximum principle.

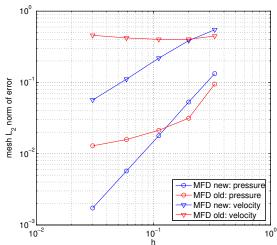
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#### References

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A polyhedral mesh (top picture) where the mixed finite element method can not be used. Note that 68% of interior mesh faces are non-planar. The convergence graphs (bottom picture) for the same problem as above show optimal convergence rates for the new MFD method (blue) and lack of convergence for the old MFD method (red).

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